Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.88

Global applicability domain: Inside

Local applicability domain index: 3.93e-01

Confidence level: 6.28e-01

Nearest Neighbors from the Training Set

Image not found
Chlorothalonil
Measured: 3.05
Predicted: 2.88

Image not found
2,4,5-Tribromoimidazole
Measured: 1.96
Predicted: 2.43

Image not found
2-(Thiocyanomethylthio)benzothiazole
Measured: 3.30
Predicted: 2.64

Image not found
Ioxynil
Measured: 3.43
Predicted: 2.31

Image not found
4,6-Dichloro-1,3-benzothiazole-2-sulfonamide
Measured: 2.60
Predicted: 1.26